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TITLE: Determination of atomic charges in molecules by means of X-ray emission spectra

PERIODICAL: Physica status solidi, V.2, no.7, 1962, 904-922

TEXT: This paper provides a clear definition of the concept of atomic charges in molecules (ACM), which has not been done so far, and determines the ACM for some compounds from experimental data. After discussing various usages of the concept of ACM, a new definition is suggested, using the energy of the innermost atomic term as a measure for the ACM. The ground state of the central atom and that of its positive and negative ion in the gaseous state are chosen for the limiting values. Hence the principle of electro-

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Determination of atomic charges....

neutrality and charge distribution in molecules are interpreted in a new way. Using Slater's functions, an equation is derived for calculating the ACM from the shift of X-ray emission lines. Only such lines are used as are caused by transition between terms whose energy depends on the chemical bond and is not influenced by any additional factor. The known shifts in the  $K_{\alpha, \beta}$  lines of the elements of the third period in about 150 compounds are used, in conjunction with an empirical constant, to calculate the relevant ACM. These values are compared to data based upon other physical measurements, and some further connections between line shift and ACM are given. There are 1 figure and 11 tables.

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